PHYSICS AND CHEMISTRY OF MINERALS

Volume 14 1987

In Cooperation with the International Mineralogical Association (IMA)

Founding Editors: S. S. Hafner and C. T. Prewitt

Edited by I. Jackson, A.S. Marfunin, A. Navrotsky, F. Seifert

Advisory Board

T.J. Ahrens Pasadena
A. Authier Paris
V.I. Baguin Moscow
A. Baronnet Marseille
G.B. Bokij Moscow
M.E. Fleet London, Ontario
V. Gabis Orléans la Source
G.V. Gibbs Blacksburg
R. Jeanloz Berkeley
D.L. Kohlstedt Ithaca
K. Langer Berlin
G. Lehmann Münster
J.D.C. McConnell Oxford, U.K.
A.C. McLaren Canberra
N. Morimoto Kyoto
R.E. Newnham University Park
A. Preisinger Vienna
A. Putnis Cambridge, U.K.
E. Salje Cambridge, U.K.
H. Schmalzried Hannover
R.N. Schock Livermore
Y. Syono Sendai
J. Tossell College Park
V.M. Vinokurov Kazan

Springer International

Physics and Chemistry of Minerals

In Cooperation with the International Mineralogical Association (IMA)

Founded in 1977. Founding Editor: S. S. Hafner.
Volumes 1–9 (1977–1983) edited by S. S. Hafner, A. S. Marfunin, and C. T. Prewitt,
from Volume 10 (1984) by I. Jackson, A. S. Marfunin, C. T. Prewitt, F. Seifert,
from Volume 13 (1986) by I. Jackson, A. S. Marfunin, A. Navrotsky, F. Seifert

Copyright

Submission of a manuscript implies: that the work described has not been published before (except in the form of an abstract or as part of a published lecture, review, or thesis); that it is not under consideration for publication elsewhere; that its publication has been approved by all coauthors, if any, as well as by the responsible authorities at the institute where the work has been carried out; that, if and when the manuscript is accepted for publication, the authors agree to automatic transfer of the copyright to the publisher and that the manuscript will not be published elsewhere in any language without the consent of the copyright holders.

All articles published in this journal are protected by copyright, which covers the exclusive rights to reproduce and distribute the article (e.g., as offprints), as well as all translation rights. No material published in this journal may be reproduced photographically or stored on microfilm, in electronic data bases, video disks, etc., without first obtaining written permission from the publisher.

The use of general descriptive names, trade names, trademarks, etc., in this publication, even if not specifically identified, does not imply that these names are not protected by the relevant laws and regulations.

While the advice and information in this journal is believed to be true and accurate at the date of its going to press, neither the authors, the editors, nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Special regulations for photocopies in the USA: Photocopies may be made for personal or in-house use beyond the limitations stipulated under Section 107 or 108 of U.S. Copyright Law, provided a fee is paid. This fee is US $ 0.20 per page, or a minimum of US $ 1.00 if an article contains fewer than five pages. All fees should be paid to the Copyright Clearance Center, Inc., 21 Congress Street, Salem, MA 01970, USA, stating the ISSN 0342-1791, the volume, and the first and last page numbers of each article copied. The copyright owner's consent does not include copying for general distribution, promotion, new works, or resale. In these cases, specific written permission must first be obtained from the publisher.

Printed by Universitätsdruckerei H. Stürtz AG, Würzburg

© Springer-Verlag Berlin Heidelberg 1987

Printed in Germany

Author Index, Volume 14

Abdullin RS, Kal'chev VP, Pen'kov IN: Investigation of Copper Minerals by NQR: Crystallochemistry, Electronic Structure, Lattice Dynamics 258–263
Akaogi M, Navrotsky A: Calorimetric Study of High-pressure Phase Transitions Among the $CdGeO_3$ Polymorphs (Pyroxenoid, Garnet, Ilmenite, and Perovskite Structures) 435–440
Akaogi M, see Matsui M, et al. 101–106
Anderson OL, see Yamamoto S 332–340
Andreoni W, Galli G: Unified Structural Classification of AB_2 Molecules and Solids from Valence Electron Orbital Radii 389–395
Armbruster Th, see Lager GA, et al. 177–180
Beran A: OH Groups in Nominally Anhydrous Framework Structures: An Infrared Spectroscopic Investigation of Danburite and Labradorite 441–445
Boggs JE: Accurate Determination of Molecular Structure and Vibrational Force Constants by Computation 407–412
Boisen MB, Jr., Gibbs GV: A Method for Calculating Fractional s-Character for Bonds of Tetrahedral Oxyanions in Crystals 373–376
Boisen MB, Jr., see Gibbs GV, et al. 327–331
Boyer LL, see Cohen RE, et al. 294–302
Bullett DW: Applications of Atomic-Orbital Methods to the Structure and Properties of Complex Transition-Metal Compounds 485–491
Büscher R, Such KP, Lehmann G: Local Relaxations around Fe^{3+} and Cr^{3+} in Al Sites in Minerals 553–559
Buseck PR, see Otten MT 45–51
Cemic L, Kleppa OJ: High Temperature Calorimetry of Sulfide Systems. II. Standard Enthalpies of Formation of Pentlandite and Violarite 52–57
Chatterjee ND, see Rimbach H 560–569
Chelikowsky JR, Chou MY: Pseudopotential Approaches to the Structural Energies of Crystalline Solids and Solid Surfaces 308–314
Chou MY, see Chelikowsky JR 308–314
Cohen RE, Boyer LL, Mehl MJ: Theoretical Studies of Charge Relaxation Effects on the Statics and Dynamics of Oxides 294–302
Couty R, see Velde B, et al. 345–349
Cox DE, see Ghose S, et al. 36–44
Czank M, see Seifert F, et al. 26–35
Dal Negro A, see Rossi G, et al. 514–520
Dang N Van, see Ghose S, et al. 36–44
Dasgupta S, see Ghosh D, et al. 151–155
Davoli I, Paris E, Mottana A, Marcelli A: Xanes Analysis on Pyroxenes with Different Ca Concentration in M2 Site 21–25
Dowty E: Fully Automated Microcomputer Calculation of Vibrational Spectra 67–79
Dowty E: Vibrational Interactions of Tetrahedra in Silicate Glasses and Crystals: I. Calculations on Ideal Silicate-Aluminate-Germanate Structural Units 80–93
Dowty E: Vibrational Interactions of Tetrahedra in Silicate Glasses and Crystals: II. Calculations on Melilites, Pyroxenes, Silica Polymorphs and Feldspars 122–138
Dowty E: Vibrational Interactions of Tetrahedra in Silicate Glasses and Crystals. III. Calculations on Simple Sodium and Lithium Silicates, Thortveitite and Rankinite 542–552
Editorial Statement 293
Ellis DE: Vacancy and Defect Structures in Metal Oxides 303–307
Ender A, see Srečec I, et al. 492–498
Eriksson G, see Srečec I, et al. 492–498
Fabrichnaya OB, see Kuskov OL 58–66
Ferrow E: Mössbauer and X-ray Studies on the Oxidation of Annite and Ferriannite 270–275
Ferrow E: Mössbauer Effect and X-ray Diffraction Studies of Synthetic Iron Bearing Trioctahedral Micas 276–280
Finger LW, see Gibbs GV, et al. 327–331
see Hazen RM 426–434
FitzGerald JD, see McLaren AC 281–292
Flörke OW, see Graetsch H, et al. 249–257
Fornes V, see Ocaña M, et al. 527–532
Fyfe CA, see Putnis A, et al. 446–454
Galli G, see Andreoni W 389–395
Gans W, see Srečec I, et al. 492–498
Garcia-Ramos JV, see Ocaña M, et al. 527–532
Ghose S, Cox DE, Dang N Van: Magnetic Order in Grunerite, $Fe_7Si_8O_{22}(OH)_2$ – A Quasi-One Dimensional Antiferromagnet with a Spin Canting Transition 36–44
Ghose S, see Ghosh D, et al. 151–155
Ghosh D, Kundu T, Dasgupta S, Ghose S: Electron Delocalization and Magnetic Behavior in a Single Crystal of Ilvaite, a Mixed Valence Iron Silicate 151–155
Gibbs GV, Finger LW, Boisen MB, Jr.: Molecular Mimicry of the Bond Length-Bond Strength Variations in Oxide Crystals 327–331
Gibbs GV, see Boisen MB, et al. 373–376
see Lasaga AC 107–117
see Spackmann MA, et al. 139–150
Gordon RG, see Hemley RJ, et al. 2–12
Graetsch H, Flörke OW, Miehe G: Structural Defects in Microcrystalline Silica 249–257
Hargittai I, see Hargittai M 413–425
Hargittai M, Hargittai I: Gas-Solid Molecular Structure Differences 413–425
Harlow GE, see Miller GH, et al. 461–472
Hayashi M, Tamura I, Shimomura O, Sawamoto H, Kawamura H: Antiferromagnetic Transition of Fayalite under High Pressure Studied by Mössbauer Spectroscopy 341–344
Hazen RM: High-Pressure Crystal Chemistry of Chrysoberyl, Al_2BeO_4: Insights on the Origin of Olivine Elastic Anisotropy 13–20
Hazen RM, Finger LW: High-Temperature Crystal Chemistry of Phenakite (Be_2SiO_4) and Chrysoberyl ($BeAl_2O_4$) 426–434
Hemley RJ, Jackson MD, Gordon RG: Theoretical Study of the Structure, Lattice Dynamics, and Equations of State of Perovskite-type $MgSiO_3$ and $CaSiO_3$ 2–12
Henrich VE: Electron Spectroscopic Studies of Perfect and Defect Metal Oxide Surfaces 396–400
Hill RJ, see Spackmann MA, et al. 139–150
Hoering TC, see Hofmeister AM, et al. 205–224
Hofmeister AM: Single-Crystal Absorption and Reflection Infrared Spectroscopy of Forsterite and Fayalite 499–513
Hofmeister AM, Hoering TC, Virgo D: Vibrational Spectroscopy of Beryllium Aluminosilicates: Heat Capacity Calculations from Band Assignments 205–224
Ito E, see Kudoh Y, et al. 350–354
Jackson MD, see Hemley RJ, et al. 2–12
Jacobsson E, see Srečec I, et al. 492–498
Kal'chev VP, see Abdullin RS, et al. 258–263
Karato S: Scanning Electron Microscope Observation of Dislocations in Olivine 245–248
Kawamura H, see Hayashi M, et al. 341–344
Kikuchi M, see Velde B, et al. 345–349
Kleppa OJ, see Cemic L 52–57
Kudoh Y, Ito E, Takeda H: Effect of Pressure on the Crystal Structure of Perovskite-Type $MgSiO_3$ 350–354
Kundu T, see Ghosh D, et al. 151–155
Kuskov OL, Fabrichnaya OB: The SiO_2 Polymorphs: The Equations of State and Thermodynamic Properties of Phase Transformations 58–66
Lager GA, Armbruster Th, Pohl D: Prediction of Refractive Indices in Minerals from Crystallographic Data: Applications and Limitations of the Point-Dipole Model 177–180
Lasaga AC, Gibbs GV: Applications of Quantum Mechanical Potential Surfaces to Mineral Physics Calculations 107–117
Le Bail C, Thomassin JH, Touray JC: Hydrotalcite-Like Solid Solutions with Variable SO_4^{2-} and CO_3^{2-} Contents at 50° C. An X-Ray Diffraction and Raman Spectrometry Study 377–382
Lehmann G, see Büscher R, et al. 553–559
see Plath I 383–386
Lofgren GE, see McCormick TC, et al. 368–372
Marcelli A, see Davoli I, et al. 21–25
Mason TO: Cation Intersite Distributions

in Iron-Bearing Minerals Via Electrical Conductivity/Seebeck Effect 156–162
Matsui M, Akaogi M, Matsumoto T: Computational Model of the Structural and Elastic Properties of the Ilmenite and Perovskite Phases of $MgSiO_3$ 101–106
Matsumoto T, see Matsui M, et al. 101–106
Mattson SM, Rossman GR: Fe^{2+}-Fe^{3+} Interactions in Tourmaline 163–171
Mattson SM, Rossman GR: Identifying Characteristics of Charge Transfer Transitions in Minerals 94–99
McCormick TC, Smyth JR, Lofgren GE: Site Occupancies of Minor Elements in Synthetic Olivines As Determined by Channeling-Enhanced X-ray Emission 368–372
McLaren AC, FitzGerald JD: CBED and ALCHEMI Investigation of Local Symmetry and Al, Si Ordering in K-feldspars 281–292
McMillan PF, Ross NL: Heat Capacity Calculations for Al_2O_3 Corundum and $MgSiO_3$ Ilmenite 225–234
Mehl MJ, see Cohen RE, et al. 294–302
Mellini M, see Rossi G, et al. 514–520
Miehe G, see Graetsch H, et al. 249–257
Miller GH, Rossman GR, Harlow GE: The Natural Occurrence of Hydroxide in Olivine 461–472
Molin GM, see Rossi G, et al. 514–520
Mottana A, see Davoli I, et al. 21–25
Müller WF, Vojdan-Shemshadi Y, Pentinghaus H: Transmission Electron Microscopic Study of Antiphase Domains in $CaAl_2Ge_2O_8$-Feldspar 235–237
Murad E, Wagner FE: The Mössbauer Spectrum of Almandine 264–269
Navrotsky A, see Akaogi M 435–440
see Ross NL 473–481
Oberti R, see Rossi G, et al. 514–520
Ocaña M, Fornes V, Garcia-Ramos JV, Serna CJ: Polarization Effects in the Infrared Spectra of α-Quartz and α-Cristobalite 527–532
Otten MT, Buseck PR: The Oxidation State of Ti in Hornblende and Biotite Determined by Electron Energy-Loss Spectroscopy, with Inferences Regarding the Ti Substitution 45–51
Özkan H, see Tatli A 172–176
Paris E, see Davoli I, et al. 21–25
Pen'kov IN, see Abdullin RS, et al. 258–263
Pentinghaus H, see Müller WF, et al. 235–237
Petersen N, Schembera N, Schmidbauer E, Vali H: Magnetization, Mössbauer Spectroscopy and Structural Studies of a Ferrimagnetic Fe-Oxide Formed by Heating Nontronite in Air 118–121
Plath I, Lehmann G: Thermoluminescence of Shock-Loaded Amethyst Quartz 383–386
Pohl D, see Lager GA, et al. 177–180
Putnis A, Salje E, Redfern SAT, Fyfe CA, Strobl H: Structural States of Mg-Cordierite I: Order Parameters from Synchrotron X-Ray and NMR Data 446–454
Redfern SAT, Salje E: Thermodynamics of Plagioclase II: Temperature Evolution of the Spontaneous Strain at the $I\bar{1} \leftrightarrow P\bar{1}$ Phase Transition in Anorthite 189–195
Redfern SAT, see Putnis A, et al. 446–454
Ricoult DL, Schmalzried H: Internal Reduction of (Mg, Ni)O: Effect of a NiO-Concentration Gradient 238–244
Rimbach H, Chatterjee ND: Equations of State for H_2, H_2O, and H_2-H_2O Fluid Mixtures at Temperatures Above 0.01° C and at High Pressures 560–569
Rosén E, see Srečec I, et al. 492–498
Ross NL, Navrotsky A: The Mg_2GeO_4 Olivine-Spinel Phase Transition 473–481
Ross NL, see McMillan PF 225–234
Rossi G, Oberti R, Dal Negro A, Molin GM, Mellini M: Residual Electron Density at the *M2* Site in *C2/c* Clinopyroxenes: Relationships with Bulk Chemistry and Sub-Solidus Evolution 514–520
Rossman GR, see Mattson SM 94–99, 163–171
see Miller GH, et al. 461–472
Runciman WA: Electron Density and Polarized Absorption Spectra of Fayalite: *A Comment* 387
Runciman WA: The Spin-Forbidden Absorption Spectrum of Fe^{2+} in Orthopyroxene: *A Comment* 482
Salje E: Structural States of Mg-Cordierite II: Landau Theory 455–460
Salje E: Thermodynamics of Plagioclases I: Theory of the $I\bar{1}-P\bar{1}$ Phase Transition in Anorthite and Ca-rich Plagioclases 181–188
Salje E, see Putnis A, et al. 446–454
see Redfern SAT 189–195
Sawamoto H, see Hayashi M, et al. 341–344
Schembera N, see Petersen N, et al. 118–121
Schmahl W, see Seifert F, et al. 26–35
Schmalzried H, see Ricoult DL 238–244
Schmidbauer E: ^{57}Fe Mössbauer Spectroscopy and Magnetization of Cation-Deficient Fe_2TiO_4 and $FeCr_2O_4$. Part I: ^{57}Fe Mössbauer Spectroscopy 533–541
Schmidbauer E, see Petersen N, et al. 118–121
Schwarz K: Band Theoretical Studies of the Electronic Structure of Oxides 315–319
Seifert F, Czank M, Simons B, Schmahl W: A Commensurate-Incommensurate Phase Transition in Iron-Bearing Åkermanites 26–35
Serna CJ, see Ocaña M, et al. 527–532
Sherman DM: Molecular Orbital (SCF-Xα-SW) Theory of Metal-Metal Charge Transfer Processes in Minerals. I. Application to $Fe^{2+} \rightarrow Fe^{3+}$ Charge Transfer and "Electron Delocalization" in Mixed-Valence Iron Oxides and Silicates 355–363
Sherman DM: Molecular Orbital (SCF-Xα-SW) Theory of Metal-Metal Charge Transfer Processes in Minerals. II. Application to $Fe^{2+} \rightarrow Ti^{4+}$ Charge Transfer Transitions in Oxides and Silicates 364–367
Shimomura O, see Hayashi M, et al. 341–344
Simons B, see Seifert F, et al. 26–35
Skogby H: Kinetics of Intracrystalline Order-Disorder Reactions in Tremolite 521–526
Smyth JR, see McCormick TC, et al. 368–372
Spackmann MA, Hill RJ, Gibbs GV: Exploration of Structure and Bonding in Stishovite with Fourier and Pseudoatom Refinement Methods Using Single Crystal and Powder X-ray Diffraction Data 139–150
Srečec I, Ender A, Woermann E, Gans W, Jacobsson E, Eriksson G, Rosén E: Activity-Composition Relations of the Magnesiowüstite Solid Solutions Series in Equilibrium with Metallic Iron in the Temperature Range 1050–1400 K 492–498
Stoneham AM: Quantitative Modelling of Defect Processes in Ionic Crystals 401–406
Strobl H, see Putnis A, et al. 446–454
Such KP, see Büscher R, et al. 553–559
Sunagawa I, see Yada K, et al. 197–204
Syono Y, see Velde B, et al. 345–349
Takeda H, see Kudoh Y, et al. 350–354
Tamura I, see Hayashi M, et al. 341–344
Tanji T, see Yada K, et al. 197–204
Tatli A, Özkan H: Variation of the Elastic Constants of Tourmaline with Chemical Composition 172–176
Thomassin JH, see Le Bail C, et al. 377–382
Tossell JA: Quantum Mechanical Studies of Si–O and Si–F Bonds in Molecules and Minerals 320–326
Touray JC, see Le Bail C, et al. 377–382
Vali H, see Petersen N, et al. 118–121
Velde B, Syono Y, Couty R, Kikuchi M: High Pressure Infrared Spectra of Diaplectic Anorthite Glass 345–349
Virgo D, see Hofmeister AM, et al. 205–224
Vojdan-Shemshadi Y, see Müller WF, et al. 235–237
Wagner FE, see Murad E 264–269
Wang HS, see Zhao SB, et al. 483–484
Woermann E, see Srečec I, et al. 492–498
Yada K, Tanji T, Sunagawa I: Radiation Induced Lattice Defects in Natural Zircon ($ZrSiO_4$) Observed at Atomic Resolution 197–204
Yamamoto S, Anderson OL: Elasticity and Anharmonicity of Potassium Chloride at High Temperature 332–340
Zhao SB, Wang HS, Zhou KW: On the Approach to the Assignment of Spin-Forbidden Bands of Complex Ions: *A Reply* 483–484
Zhou KW, see Zhao SB, et al. 483–484

Subject Index, Volume 14

All mineral names occurring in titles, subtitles and abstracts are indexed. Chemical formulae are according to M. Fleischer, Glossary of Mineral Species, 1983 (in some cases simplified) or as given by the author. The numbers refer to the title page.

A

akermanite $Ca_2MgSi_2O_7$ cf. melilite group
amphibole group
  electron energy-loss spectroscopy 45
  grunerite 36
  kinetics 521
  magnetic properties 36
  magnetic structure 36
  neutron diffraction 36
  order-disorder Mg–Fe 521
  Ti oxidation state 45
  tremolite 521
anharmonicity
  sylvite 332
anorthite $CaAl_2Si_2O_8$
  diaplectic glass 345
  shock effects 345
antiphase domains
  $CaAl_2Ge_2O_8$ feldspar 235
atom location by channelling enhanced microanalysis (ALCHEMI)
  K-feldspar 281
  olivine 368

B

babingtonite $Ca_2Fe_2Si_5O_{14}OH$
  intervalence charge transfer 94
  magnetic properties 94
  optical spectra 94
backscattered electron image (BEI)
  olivine 245
bertrandite $Be_4Si_2O_7(OH)_2$
  heat capacity 205
  infrared spectrum 205
  Raman spectrum 205
beryl $Be_3Al_2Si_6O_{18}$
  electron paramagnetic resonance 553
  heat capacity 205
  infrared spectrum 205
  Raman spectrum 205
bond distances
  fractional s-character 373
  hydroxyacid molecules 327
  tetrahedral oxyanions 373
bond strength
  hydroxyacid molecules 327
bromellite BeO
  elasticity 294
  equation of state 294
  heat capacity 205
  infrared spectrum 205
  lattice dynamics 294
  Raman spectrum 205

C

calorimetry
  $CdGeO_3$ polymorphs 435
  pentlandite 52
  pyrite 52
  pyrrhotite 52
  vaesite 52
  violarite 52
chalcedony SiO_2
  intergrowth structure 249
  structural defects 249
chalcocite Cu_2S
  nuclear quadrupole resonance 258
charge density
  bonding 315
  quantum calculations 315
chemical bond
  AB_2 molecules 389
  corundum 303
  fractional s-character 373
  hybridization 373
  quantum calculations 303, 308, 315, 320
  rocksalt 308
  Si–F 320
  Si–O 320, 413
  stishovite 139
  surfaces 308
  tetrahedral oxyanions 373
  wüstite 303
  zincblende 308
  zirconia 303
chemisorption
  oxides 391
chrysoberyl Al_2BeO_4
  compressibility 13
  elasticity 13
  equation of state 13, 426
  heat capacity 205
  high temperature structure 426
  high pressure structure 13
  infrared spectrum 205
  Raman spectrum 205
  thermal expansion 426
coesite SiO_2
  equation of state 58
  phase transition 58
  thermodynamic properties 58
compressibility
  chrysoberyl 13
  olivine 13
conductivity
  cation distribution from 156
  olivine 156
  spinel 156
convergent beam electron diffraction (CBED)
  K-feldspar 281
copper complexes
  nuclear quadrupole resonance 258
cordierite $(Mg,Fe)_2Al_4Si_5O_{18}$
  Al,Si ordering 446
  elastic energy 455
  electron paramagnetic resonance 553
  Landau theory 455
  modulated phase 446, 455
  phase transitions 446, 455
corundum Al_2O_3
  defect structure 303
  elasticity 294
  equation of state 294
  heat capacity 225
  lattice dynamics 294
  quantum calculations 303
cristobalite SiO_2
  defects 249
  intergrowth structure 249
  infrared spectra 527
crystal chemistry
  clinopyroxenes 514
crystal structure
  AB_2 molecules 389
  chrysoberyl high P 13
  chrysoberyl high T 426
  clinopyroxene 514
  $MgSiO_3$ perovskite-type 101, 350
  $MgSiO_3$ ilmenite type 101
  phenakite high T 426
  pressure effect 350
  stishovite 139
cubanite $CuFe_2S_3$
  nuclear quadrupole resonance 258

D

danburite $CaB_2Si_2O_8$
  infrared spectra 441
  OH groups 441
defects
  atomic resolution 197
  chalcedony 249
  corundum 303
  flint 249
  ionic crystals 401
  (Mg,Ni)O 238
  moganite 249
  olivine 245
  opal 249
  oxides 396
  quantum calculation 303, 315, 401
  radiation damage 197
  surface 396
  wüstite 303
  zircon 197
  zirconia 303
dehydrogenation
  biotite 270
density of states
  quantum calculations 315
diamond anvil cell
  structure determination 350
diaplectic glass
  anorthite 345
  infrared spectra 345

E

elastic properties
  anharmonicity 332
  bromellite 294
  chrysoberyl 13
  cordierite 455
  corundum 294
  energy 455
  forsterite 13
  high temperature effects 332
  ilmenite-type $MgSiO_3$ 101
  olivine 13
  orthosilicates 107
  periclase 294
  perovskite-type $MgSiO_3$ 101
  quartz 294
  rutile 294
  silica polymorphs 107
  stishovite 294
  sylvite 332
  tourmaline 172
electron channelling
  K-feldspar 281
  olivine 368
electron delocalization
  ilvaite 151, 355
  magnetite 355
  MO theory 355
electron density
  fayalite 387
electron diffraction
  melilite 26
electron energy-loss spectroscopy
  Ti oxidation state biotite, hornblende 45
electronic structure
  tetrahedrite 485
electron gas model
  silicate perovskite 2
electron hopping
  ilvaite 355
  magnetite 355
  MO theory 355
electron microscopy
  atomic resolution 197
  $CaAl_2Ge_2O_8$ feldspar 235
  chalcedony 249
  flint 249

melilite 26
modulated structure 26
moganite 249
olivine 245
opal 249
radiation induced lattice defects 197
zircon 197
electron paramagnetic resonance (EPR)
beryl 553
cordierite 553
local relaxation 553
scolecite 553
superposition model 553
electronic charge transfer
between iron cations 163, 355
babingtonite 94
euclase 94
Fe–Ti 364
lazulite 94
magnetite 355
optical absorption spectra 364
rockbridgeite 94
tourmaline 163
emf-measurements
magnesiowüstite 492
enthalpy
sulfides 52
equation of state
bromellite 294
$CaSiO_3$ perovskite 2
chrysoberyl 13, 426
coesite 58
corundum 294
H_2 560
H_2O 560
H_2-H_2O fluid mixtures 560
$MgSiO_3$ perovskite 2, 350
olivine 13
periclase 294
phenakite 426
quartz 58, 294
rutile 294
stishovite 58, 294
sylvite 332
euclase $BeAlSiO_4OH$
heat capacity 205
infrared spectrum 205
intervalence charge transfer 94
optical spectra 94
Raman spectrum 205

F

far infrared spectroscopy (FIR)
olivine 499
feldspar group
$CaAl_2Ge_2O_8$ 235
calculated infrared spectra 122
calculated Raman spectra 122
fluid mixtures
equation of state H_2-H_2O 560
force constants
vibrational, computation 407

G

garnet group
almandine 264
$CdGeO_3$ garnet 435
magnetic structure 264
nuclear gamma ray resonance 264
germanate
$CaAl_2Ge_2O_8$ feldspar 235
$CdGeO_3$ 435
Gibbs-Duhem integration
ternary 429
grunerite $Fe_7Si_8O_{22}(OH)_2$
cf. amphibole group

H

halite NaCl
bonding 308
high pressure transition 308
quantum calculation 308
surfaces 308
heat capacity
bertrandite 205
beryl 205
bromellite 205
chrysoberyl 205
corundum 225
euclase 205
ilmenite-type $MgSiO_3$ 225
olivine 499
phenakite 205
high pressure
antiferromagnetic phase transition fayalite 341
$CdGeO_3$ 435
chrysoberyl 13
infrared spectra 345
nuclear gamma ray resonance 341
olivine 13
phase transition 308
rocksalt 308
zincblende 308
hybridization
bonding tetrahedral oxyanions 373
hydrotalcite $(Mg_3Al(OH)_8)_2CO_3 \cdot 2H_2O$
anion partitioning 377
Raman spectra 377
solid solutions 377
hydroacid molecules
bond length 327
bond strength 327
hydroxyl groups
danburite 441
humite 461
labradorite 441
olivine 461

I

ilmenite type
calorimetry 435
$CdGeO_3$ 435
crystal structure 101
elasticity 101
$MgSiO_3$ 101, 225
phase transitions 435
potential energy model 101
thermodynamic properties 225
ilvaite $CaFe_2^{+2}Fe^{+3}(SiO_4)_2(OH)$
electron hopping 355
intervalence charge transfer 151, 355
magnetic anisotropy 151
magnetic structure 151
phase transition crystallographic 151
phase transition magnetic 151
rotation of molar susceptibility 151
incommensurate structure
melilite 26
infrared absorption (IR) spectra
cf. also far infrared spectra
bertrandite 205
beryl 205
bromellite 205
calculation 67, 80, 122, 542
chrysoberyl 205
cristobalite 527
danburite 441
diaplectic anorthite glass 345
euclase 205
fayalite 499
feldspar 122, 441
forsterite 499
high pressure 345
humite 461
hydroxyl groups 441, 461
lithium silicates 542
melilite 122
Na silicates 542
olivine 461, 499
phenakite 205
polarized 441
pyroxenes 122
quartz 527
rankinite 542
shape effects 527
thortveitite 542
tridymite 122
interatomic potential
ionic crystals 401
quantum calculations 401
intergrowth structure
chalcedony 249
flint 249
opal 249
intermolecular interaction 414
internal reduction
(Mg,Ni)O 238

K

kinetics
cation ordering tremolite 521
transport (Mg,Ni)O 238

L

Landau theory
phase transitions anorthite 181
phase transitions cordierite 455
lattice dynamics
bromellite 294
$CaSiO_3$ perovskite 2
copper complexes 258
corundum 294
$MgSiO_3$ perovskite 2
periclase 294
quartz 294
rutile 294
stishovite 294
lattice vibration
Mg_2GeO_4 olivine, spinel 473
lazulite $MgAl_2(PO_4)_2(OH)_2$
intervalence charge transfer 94
optical spectra 94
Li silicates
vibrational spectra 542

M

magnesiowüstite (Mg,Fe)O
activity-composition relation 492
emf-measurement 492
magnetic ordering
fayalite high pressure 341
magnetic properties
babingtonite 94
fayalite 341
Fe_2O_3 118
grunerite 36
ilvaite 151
rockbridgeite 94
small particles 533
spinel 533
magnetic structure
almandine 264
grunerite 36
ilvaite 151
magnetite Fe_3O_4
electron delocalization 355
electron hopping 355
metal-metal charge transfer 355
titanomagnetite 533
melilite $(Ca,Na)_2(Mg,Fe,Al)(Si,Al)_2O_7$
akermanite-ferroakermanite 26
calculated infrared spectra 122
calculated Raman spectra 122
electron diffraction 26
incommensurate phase 26
nuclear gamma ray resonance 26
phase transition 26
metal-metal bonding
tetrahedrite 485
metal-metal charge transfer
MO theory 355
mica group
biotite 45, 270, 276
dehydrogenation 270
electron energy-loss spectroscopy 45
nuclear gamma ray resonance 270, 276
oxidation 270

oxybiotite 270
structural misfit 276
Ti oxidation state 45
microcline $KAlSi_3O_8$
Al,Si ordering 281
microstructure
chalcedony 249
clinopyroxene 514
modulated structure
cordierite 446, 455
cf. incommensurate structure
molecular cluster calculation
quantum mechanical potential surfaces 107
silicates 107
molecular orbital (MO) theory
electron delocalization 355
electron hopping 355
Fe–Ti charge transfer 364
ilvaite 355
magnetite 355
metal-metal charge transfer 355
optical spectra 364
molecular shapes
AB_2 molecules 389
molecular structure
computation 407
metal halides 413
sulfones 413
montmorillonite group
ferrimagnetic Fe-oxide 118
nontronite 118
nuclear gamma ray resonance 118
morphology
internal reduction (Mg,Ni)O 238
Mössbauer spectroscopy
cf. nuclear gamma ray resonance (NGR)

N

Na silicates
vibrational spectra 542
neutron diffraction
grunerite 36
normal-coordinate
calculation of vibrational spectra 67, 80, 122
nuclear gamma ray resonance (NGR)
almandine 264
antiferromagnetic transition 341
biotite 270, 276
fayalite 341
ferrimagnetic Fe oxide 118
high pressure 341
melilites, Fe^{2+} 26
oxybiotite 270
small particles 533
spinel 533
titanomagnetite 533
nuclear quadrupole resonance (NQR)
chalcocite 258
chalcopyrite 258
cubanite 258
skinnerite 258
wittichenite 258

O

olivine group
antiferromagnetic transition, pressure 341
backscattered electron image 245
band assignment 499
cation distribution 156, 368
conductivity 156
deformation 461
dislocation 245
elastic properties 13
electron channelling 368
fayalite 341
heat capacity 499
hydroxyl groups 461
infrared spectroscopy 461, 499
lattice vibrations 473
Mg_2GeO_4 473
optical absorption spectra 387
scanning electron microscopy 245
Seebeck effect 156
spinel transition 473
opal $SiO_2 \cdot nH_2O$
defects 249
intergrowth structure 249
optical absorption spectra
babingtonite 94
band intensities 163
euclase 94
fayalite 387
Fe–Ti charge transfer 364
intervalence charge transfer 94, 163
lazulite 94
orthopyroxene 482, 483
rockbridgeite 94
spin-forbidden spectrum 482, 483
tourmaline 163
optical properties
predicted by point-dipole model 177
order-disorder
by atom location by channelling enhanced microanalysis 281, 368
by conductivity – Seebeck effect 156
by convergent beam electron diffraction 281
cordierite: Si,Al 446
cooling rate 521
kinetics 521
Mg_2GeO_4:Mg,Ge 473
microcline: Si,Al 281
olivine 156, 368
orthoclase: Si,Al 281
sanidine: Si,Al 281
spinel group 156
tremolite: Mg,Fe 521
orthoclase $KAlSi_3O_8$
Si,Al order 281
oxidation
activation energy 270
biotite 270
dehydrogenation 270
transition state biotite 270
oxidation state
Ti by electron energy-loss spectroscopy 45
Ti in biotite, hornblende 45

P

pentlandite $Fe_{4.5}Ni_{4.5}S_8$
enthalpy 52
periclase MgO
elastic constants 294
equation of state 294
lattice dynamics 294
perovskite type
calorimetry 435
$CaSiO_3$ 2
$CdGeO_3$ 435
crystal structure 101, 350
elasticity 101
electron gas model 2
equation of state 2, 350
lattice dynamics 2
$MgSiO_3$ 2, 101, 350
phase transition 435
potential energy model 101
phase transition
anorthite 181, 188
antiferromagnetic-paramagnetic 341
$CdGeO_3$ 435
coesite 58
cordierite 446, 455
elastic energy 455
fayalite 341
germanates 435
garnet-ilmenite type $CdGeO_3$ 435
high pressures 308, 341, 435
ilmenite-perovskite type $CdGeO_3$ 435
ilvaite 151
Landau theory 455
magnetic 151
melilite 26
Mg_2GeO_4 473
modulated phases 26, 455
olivine-spinel 473
plagioclase 181, 189
pyroxene-ilmenite type $MgSiO_3$ 225
pyroxenoid-garnet type $CdGeO_3$ 435
quantum calculation 308
quartz 58
rocksalt 308
stishovite 58
zincblende 308
phenakite Be_2SiO_4
crystal chemistry 426
equation of state 426
heat capacity 205
high-temperature structure 426
infrared spectrum 205
Raman spectrum 205
thermal expansion 426
plagioclase $(Na,Ca)Al(Al,Si)Si_2O_8$
anorthite 181, 189, 345
diaplectic glass 345
infrared spectra 441
labradorite 441
Landau theory 181
lattice parameters 189
OH groups 441
phase transformations 181, 189
shock effects 345
spontaneous strain 189
point dipole model
applications to refractive index calculations 177
polarizability
electronic 177
potential energy model
ilmenite-type $MgSiO_3$ 101
perovskite-type $MgSiO_3$ 101
potential surfaces
by quantum mechanics 108
molecular clusters 107
pseudoatom refinement method
stishovite 139
pseudopotential
quantum calculations 308
pyrite FeS_2
enthalpy 52
pyroxene group
clinopyroxenes 514
crystal structure 21, 514
diopside 21
infrared spectra 122
jadeite 21, 122
microstructures 514
optical absorption spectra 482, 483
orthopyroxene 482, 483
Raman spectra 122
residual electron density 514
spodumene 122
transformation ilmenite-type $MgSiO_3$ 225
X-ray spectra (Ca) 21
pyroxenoid group
transformation garnet-type $CdGeO_3$ 435
pyrrhotite $Fe_{1-x}S$
enthalpy 52

Q

quantum calculations
bonding 308, 315, 320
charge density 315
defect structures 303, 315, 401
high pressure transitions 308
ionic crystals 401
surfaces 308
quantum mechanics
potential surfaces 107
molecular clusters 107
quartz SiO_2
amethyst 383
defects 249
elastic properties 294
equation of state 58, 294
infrared spectra 527

intergrowth structure 249
lattice dynamics 294
phase transformation 58
shock effects 383
thermodynamic properties 58
thermoluminescence 383

R

radiation damage
zircon 197
Raman spectra
bertrandite 205
beryl 205
bromellite 205
calculation 67, 80, 122, 533
chrysoberyl 205
euclase 205
hydrotalcite 377
Li silicates 542
melilite 122
Mg_2GeO_4 spinel 473
Na silicates 542
phenakite 205
pyroxenes 122
rankinite 542
thortveitite 542
tridymite 122
rankinite $Ca_3Si_2O_7$
vibrational spectra 542
relaxation
Cr^{3+} 553
electron paramagnetic resonance 553
Fe^{3+} 553
local 553
residual electron density
clinopyroxenes 514
rockbridgeite $(Fe,Mn)Fe_4(PO_4)_3(OH)_5$
intervalence charge transfer 94
magnetic properties 94
optical absorption spectra 94
rutile group
elastic properties 294
equation of state 294
lattice dynamics 294

S

sanidine $KAlSi_3O_8$
Al,Si order 281
Seebeck effect
cation distribution from 156
olivine 156
spinel 156
shape effect
infrared spectra 527
shock effects
amethyst 383
plagioclase 345
quartz 383
thermoluminescence 383
skinnerite Cu_3SbS_3
nuclear quadrupole resonance 258
solid solution thermodynamics
magnesiowüstite 492
spin canting
grunerite 36
spin-forbidden bands
orthopyroxene 482, 483
spinel group
cation deficient 533
cation distribution 156
lattice vibrations 473
magnetic properties 533
Mg_2GeO_4 473
nuclear gamma ray resonance 533
order-disorder 473
phase transition 473
Raman spectra 473
Seebeck effect 156
thermodynamic properties 473
stishovite SiO_2
bonding 139
elasticity 294
equation of state 58, 294
lattice dynamics 294
phase transition 58
structure 139
thermodynamic properties 58
structure
molecular, computation 407
molecular, metal halides 413
superposition model
electron paramagnetic resonance 553
surface
quantum calculation 308
surface structure
defects 396
electronic 396
oxides 396
sylvite KCl
anharmonicity 332
elasticity 332
equation of state 332

T

tetrahedrite $(Cu,Fe)_{12}Sb_4S_{13}$
electronic structure 485
metal-metal bonding 485
thermal expansion
chrysoberyl 426
phenakite 426
thermodynamic properties
anorthite 181
$CdGeO_3$ 435
coesite 58
H_2 560
H_2O 560
H_2-H_2O fluid mixtures 560
Landau theory 181
Mg_2GeO_4 473
olivine 473
pentlandite 52
plagioclase 181
pyrite 52
pyrrhotite 52
quartz 58
spinel 473
stishovite 58
vaesite 52
violarite 52
thermoluminescence (TL)
amethyst 383
quartz 383
shock effects 383
thortveitite $(Sc,Y)_2Si_2O_7$
vibrational spectra 542
titanium
oxidation state in biotite, hornblende 45
tourmaline
elastic properties 172
ferric iron 163
intervalence charge transfer 163
optical spectra 163
tremolite $Ca_2Mg_5Si_8O_{22}(OH)_2$
cf. amphibole group
tridymite SiO_2
defects 249
infrared spectrum 122
intergrowth structure 249
Raman spectrum 122

V

vaesite NiS_2
enthalpy 52
vibrational spectra
calculation 67, 80, 122, 407, 533
cf. infrared spectra, Raman spectra
violarite Ni_2FeS_4
enthalpy 52

W

water
equation of state 560
in danburite 441
in olivine 461
in plagioclase 441
wittichenite Cu_3BiS_4
nuclear quadrupole resonance 258
wüstite FeO
bonding 303
defects 303
quantum calculations 303
cf. magnesiowüstite
wüstite-type
internal reduction 238
(Mg,Ni)O 238
morphology 238
point defects 238
transport kinetics 238

X

X-ray spectra
diopside 21
jadeite 21
XANES 21

Z

zeolite
scolecite 553
zincblende ZnS
bonding 308
high pressure transition 308
quantum calculation 308
surface 308
zircon $ZrSiO_4$
defects 197
electron microscopy 197
fission tracks 197
radiation damage 197
ZrO_2
bonding 303
defect structure 303
quantum calculations 303